Final Report – Improvements in Neutronics/Thermal-Hydraulics Coupling in Two-Phase Flow Systems Using Stochastic-Mixture Transport Models

DOE Project DE-FC07-00ID13961

Principal Investigator: Todd S. Palmer, Oregon State University
Co-Principal Investigator: Qiao Wu, Oregon State University

Report Period: June 1, 2000 – April 30, 2003

Project Summary

In this NEER project, researchers from Oregon State University have investigated the limitations of the treatment of two-phase coolants as a *homogeneous* mixture in neutron transport calculations. Improved methods of calculating the neutron distribution in binary stochastic mixtures have been developed over the past 10-15 years and are readily available in the transport literature. These methods are computationally more expensive than the homogeneous (or atomic mix) models, but can give much more accurate estimates of ensemble average fluxes and reaction rates provided statistical descriptions of the distributions of the two materials are known. A thorough review of the two-phase flow literature has been completed and the relevant mixture distributions have been identified. Using these distributions, we have performed Monte Carlo criticality calculations of fuel assemblies to assess the accuracy of the atomic mix approximation when compared to a resolved treatment of the two-phase coolant. [Appendix A contains a summary of this work accepted for publication to the PHYSOR 2002 conference in Seoul, South Korea.] To understand the benefit of more advanced binary stochastic mixture models, we have also compared Levermore-Pomraning BSM transport calculations to atomic mix and benchmark calculations in mixtures of a material in a near void. These comparisons yield valuable information about both the ensemble average scalar flux and the variance in the scalar flux.

Phase 1 Summary of Objectives and Accomplishments

Phase 1 of the project, performed in the first project year, addressed two objectives: determine the relevant thermal hydraulic parameters describing the degree of heterogeneity for different flow regimes, and compare benchmark and atomic mix simulation results to evaluate the importance of coolant heterogeneity in the neutronic behavior of fuel assemblies. The primary goal of the first year of the project was to develop an understanding of the limitations of atomic mix applied to two-phase steam/water mixtures. The specific tasks and accomplishments associated with each objective are outlined below.

Objective 1: Determine the relevant thermal hydraulic parameters describing the degree of heterogeneity for different flow regimes.

Accomplishments: The thermal hydraulic parameters describing the degree of heterogeneity for different flow regimes have been determined for bubbly, slug, and annular flow regimes.
In the bubbly flow regime, bubbles are in spherical, elliptical or small cap shapes. For simplicity, a spherical bubble shape is a rational approximation that can greatly simplify the mathematical derivations. Since bubbles are highly dispersed in turbulent liquid, bubble size and space distribution are assumed to be independent of each other (experimental data of Wu et al. confirm this claim [1]). A typical distribution function is the upper-limit log-normal distribution function. However, the true distribution function depends on phase change rate, bubble nucleation mechanism, and bubble coalescence/breakage, which rely on the full solution of the two-fluid

thermal-hydraulics model with the addition of interfacial area transport equation. Unfortunately, such a model capability is not available yet. In this study, we shall take two approximate approaches. The first approach is to define an upper-limit log-normal distribution function throughout the bubbly flow regime. Subsequently, the void fraction increase due to vaporization can only boost the total bubble population. This artificial distribution function is effective in validating the proposed higher order Stochastic Mixture Transport Model, without involving the complexity of solving the fully coupled thermal-hydraulics equations. The second approach is to employ a uniform bubble size distribution that allows the mean bubble size to change in the flow direction. In this case, a one-dimensional thermal-hydraulics model can be applied along with the one-group interfacial area transport equation developed by Wu et al. [1]. The spatial variation of the distribution function is independent of the bubble size, but depends on the heating arrangement. For near saturation boiling on nuclear fuel clad surface, bubbles intend to accumulate in the center core region, resulting in a center-peaking void distribution, except in the bubble incipient region where wall-peaking void distribution presents. It can be modeled by $(1-(r/R)^n)$ without loss its generality. In the slug flow regime, bubbles are assumed to be of a lateral size close to the flow channel size. Small bubbles in the wake region are neglected. Therefore, the slug frequency plays a vital role in the analysis. Depending on the overall void fraction ($0.3<\alpha<0.8$), the slug frequency can be readily assigned in the proposed higher order Stochastic Mixture Transport Model. In the annular flow regime, a thin liquid film attaches to the pipe wall and a small amount of liquid is dispersed in the vapor core in the form of droplets. As a approximation, only the liquid film is considered and the film thickness is obtained from void fraction. A more detailed description of the results of this work in this Task is included in our NEER Year 1 Progress Report. [3]

Objective 2: Compare benchmark and atomic mix simulation results evaluate the importance of coolant heterogeneity in the neutronic behavior of fuel assemblies.

Accomplishments: In our proposal we indicated that we would investigate the impact of homogenized vs. spatially resolved two-phase coolant mixtures on neutron energy spectra and multiplication factor (k) in one and two dimensions. We instead approached the problem by modeling computing the multiplication factor in an infinite array of BWR coolant channels using the Monte Carlo neutron transport code MCNP4B. We perform two sets of calculations: "atomic mix", in which cross-sections for the coolant in the flow channel are calculated using an average number density (using the void fraction of the steam/water mixture, independent of the flow regime), and "benchmark", in which the steam/water interface is resolved and the cross sections of each phase are calculated using the density of that phase. In general, many realizations of the statistical distribution of the two-phase mixture must be generated in the benchmark case, and the results averaged over these realizations to compare properly with atomic mix. Figure 1 shows a two-dimensional slice of the geometry of the MCNP simulations, and describes one trend in our calculations: for a given number of vapor bubbles, realizations with bubbles in the narrowest part of the channel have a larger k than realizations containing bubble clusters in the central part of the channel. Figure 2 shows a slice of the MCNP geometry in which each plane of the problem contains eight bubbles, and the bubble size is varied to yield different void fractions. Because we are simulating an infinite lattice of BWR fuel pins, we reduced the enrichment of the fuel to 1% to cause the multiplication factor to be nearer to unity.

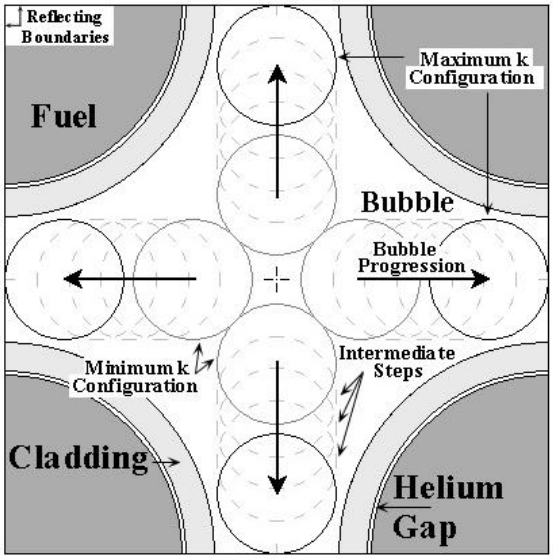
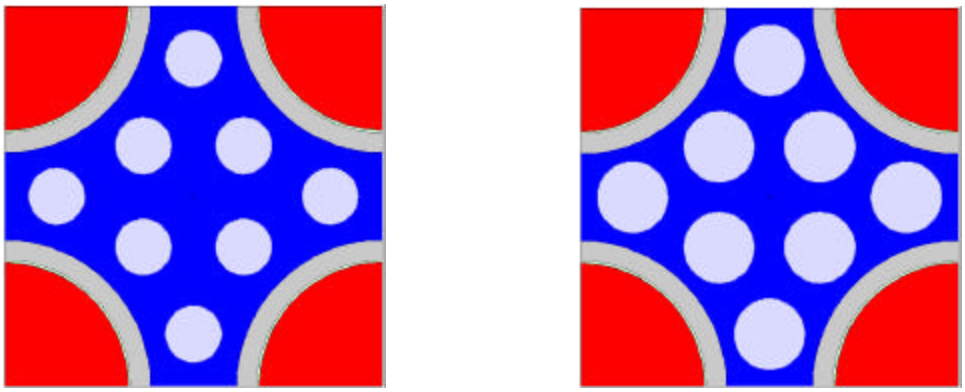
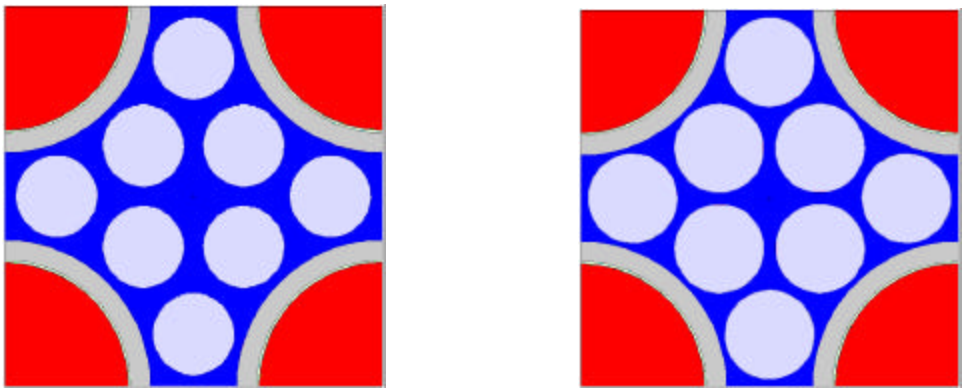


Figure 1: MCNP4B model of BWR lattice channel



(a) 10%

(b) 20%



(a) 30%

(b) 40%

Figure 2: Channel geometry with 8 bubbles and various void fractions

The detailed procedure for generating the realizations, and the complete results of these calculations can be found in our Year 1 Progress Report [3]. Our findings are that for void fractions less than 20%, 10^6 neutrons per generation, 25 skipped generations and 100 active generations, the difference in k between the atomic mix and benchmark calculations is less than or equal to the standard error in the MCNP calculation of the atomic mix k – meaning that the atomic mix approximation accurately reproduces the benchmark calculation. In the 45%-35% void range the multiplication factor calculated with resolved fluid-vapor interfaces is markedly different than that calculated by the atomic mix model; the average difference in k for any number of bubbles was \$0.74, \$0.57, and \$0.36 for 45%, 40%, and 35% void fraction, respectively. In the 30%-20% void range the difference between the two models decreases, dropping from an average of \$0.25 at 30% to \$0.12 at 25%, and then down to an average of only \$0.05 at 20% which is lost within the error range of the calculations (\$0.085).

The 30% void calculations, augmented by the calculations at other void fractions, show that the moderation properties of a coolant channel with resolved vapor-liquid interfaces are substantially different than that of an atomically mixed channel. The average difference in the calculated multiplication factor was \$0.25, which was three times higher than the standard deviation of the calculations. A summary of these results was submitted to the PHYSOR 2002 International Meeting on Reactor Physics in Seoul, South Korea [4]. Although the summary was accepted, the first author declined to submit a full paper to the conference for personal reasons.

Phase 2 Summary of Objectives and Accomplishments

Phase 2 of the project, performed in the second project year, addressed three objectives: develop two deterministic transport codes to perform benchmark (B), atomic mix (AM) and Levermore-Pomraning (LP) transport calculations, compare estimates of ensemble average neutron fluxes from the three approaches, and compare Levermore-Pomraning estimates of the variance in scalar flux to benchmark variances. The primary goal of the second year of the project is to determine if an advanced model for binary stochastic mixture transport is a significant improvement over atomic mix for two-phase coolant mixtures. In these calculations we have focused on neutron transport in the coolant mixture, and we treat it as water mixed with void. Given the density ratio of steam and water, this is a good approximation.

Objective 1: Develop two deterministic transport codes to perform benchmark, atomic mix and Levermore-Pomraning transport calculations.

Accomplishments: Our slab geometry, monoenergetic, fixed source transport codes both utilize the diamond-difference spatial discretization and the discrete ordinates approximation in angle. In our benchmark calculations, we have treated the water and void materials as Markovian (meaning the mean chord lengths in two materials have an exponential distribution) and homogeneous (meaning the distribution of material "chunk" sizes is independent of space). A Markovian distribution has recently been shown to accurately represent the distribution of chord lengths in a background material randomly populated with a second material in the form of fixed-radii disks in 2D or spheres in 3D [5]. The distribution of chords in the disks and spheres are not Markovian, but we use this approximation as a first step. Benchmark (B) calculations are performed by generating realizations of the statistical mixture given mean chord lengths (and corresponding void fractions), solving the transport equation, and then averaging the results over the realizations to compute both the ensemble average scalar flux and the variance in the scalar flux. Atomic mix (AM) calculations are performed by solving the transport equation in a single, homogenized coolant region, where the cross sections are calculated using the void fraction to

calculate the average atom density of the coolant. No information about the variance in the scalar flux is available from AM calculations. Both the benchmark and atomic mix calculations employ diffusion synthetic acceleration to efficiently iterate the transport equation to convergence. The Levermore-Pomraning (LP) binary stochastic mixture model involves two coupled transport equations for the angular flux in each of the two materials. The two equations have the form of a standard transport equation, with the added complexity of terms accounting for the transfer of particles across the interface between the two materials. Our LP code also utilizes an acceleration technique to obtain efficient solutions to these coupled equations, even for problems whose materials have drastically different neutronic properties [6]. To date, we have investigated only physical systems with no interior source, driven on one boundary by an isotropic incident angular flux, but our codes are general enough to handle a variety of boundary conditions and source configurations. In fact, these codes can be leveraged to investigate a variety of interesting binary stochastic mixture transport problems in which the background material is a void – solar radiation in cloudy atmospheres, pebble bed reactors, etc.

Objective 2: Compare estimates of ensemble average neutron fluxes from the B, AM and LP transport calculations.

Accomplishments: We have simulated a wide variety of problems to understand the range of applicability of the AM approximation, and to investigate the potential improvement in accuracy of the LP equations. We present here the results of two representative problems that show the scalar fluxes from all three methods. Figure 3 shows the scalar flux distribution in a 5 cm coolant mixture with a void fraction [$l_2/(l_1 + l_2)$] of 25% . The scattering ratio in the simulated water is 0.99, and the total cross section is 1.0 cm^{-1}. Both the AM and LP approximate transport methods predict the benchmark results very accurately. This figure also shows the variance in the benchmark calculation of the scalar flux due to the statistical nature of the mixing.

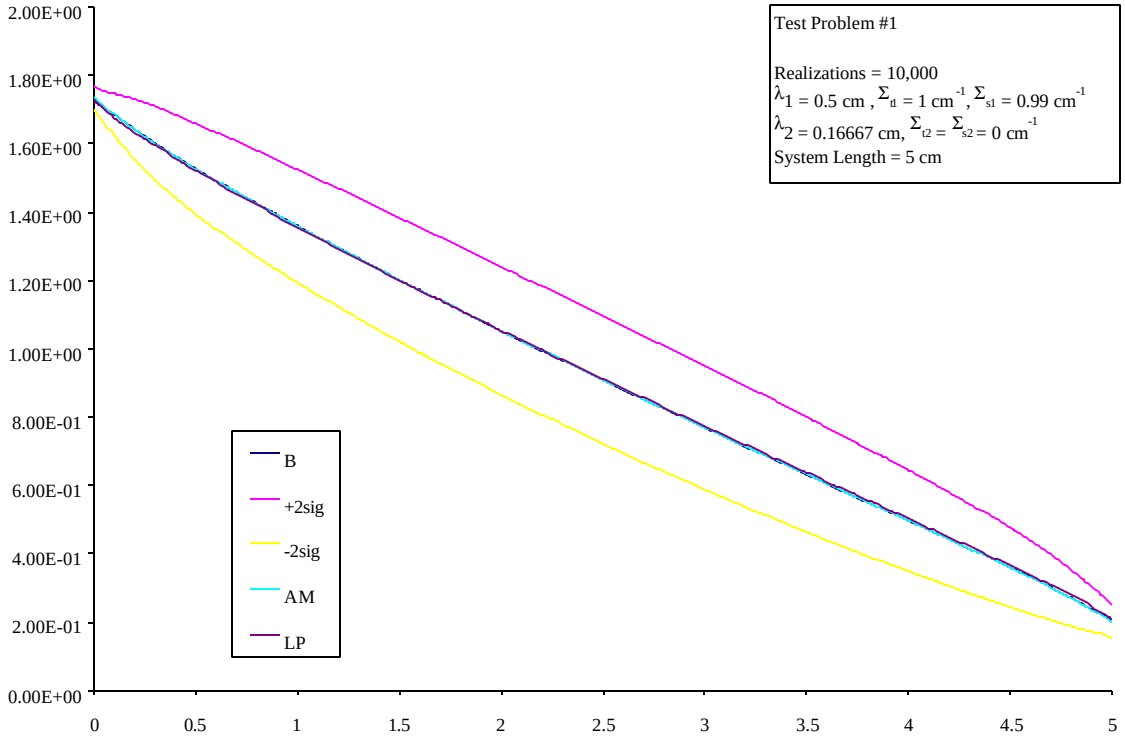


Figure 3: Scalar flux comparison for Test Problem #1

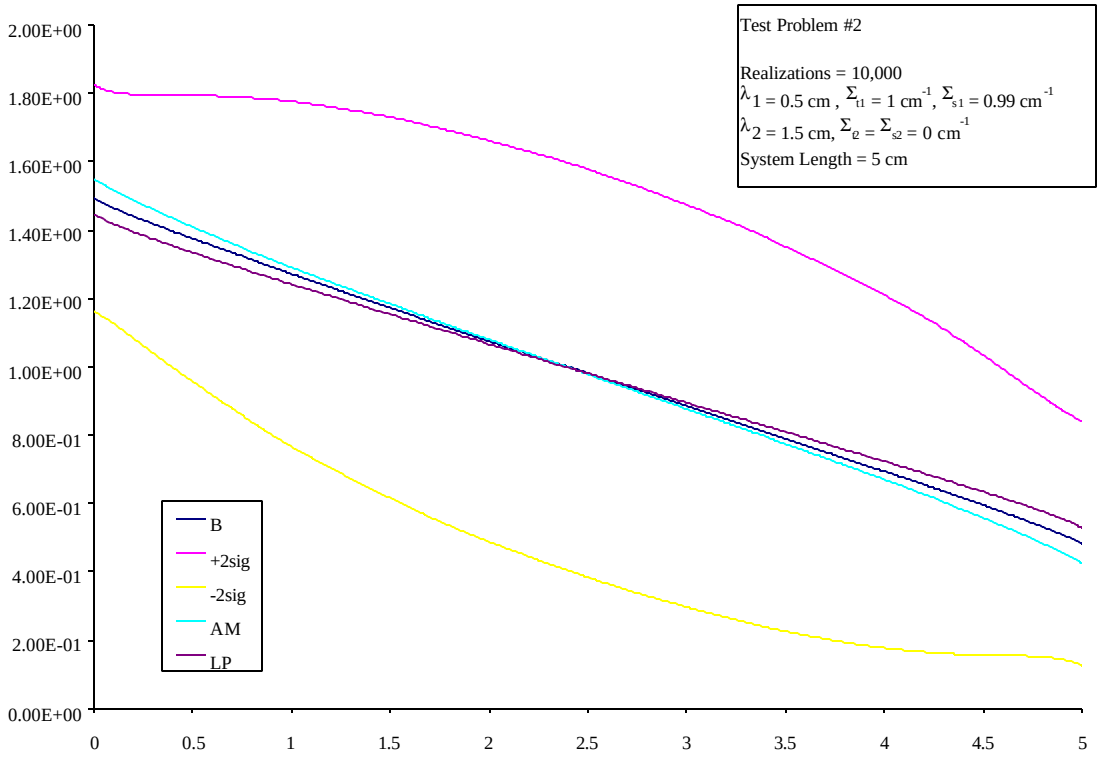


Figure 4: Scalar flux comparison for Test Problem #2

Figure 4 shows the scalar flux distribution in a 5 cm coolant mixture where the void fraction is 0.75. Both the AM and LP results differ from the benchmark results on both ends of the slab 3%, though their differences are in opposite directions. Calculations of other problems follow these trends: 1) AM predictions of the scalar flux are most inaccurate when the scattering ratio of the non-void material is in the intermediate range (0.3-0.7); 2) LP predictions of scalar flux more closely match the benchmark solutions unless the non-void material scattering ratios are very near one; 3) in general, discrepancies between the approximate methods and the benchmark calculations are more pronounced as the size of the problem (in mean free paths) increases.

Objective 3: Compare Levermore-Pomraning estimates of the variance in scalar flux to benchmark variances.

Accomplishments:

Larsen [7] has recently developed a coupled set of transport equations that can be used to estimate the variance in the scalar flux in a binary stochastic mixture. The approximation is exact if the true angular flux solution is separable in angle and space. The scalar flux variance is a very important quantity in our evaluation of the LP transport model as a possible improvement over atomic mix. A large variance in the scalar flux signifies that the inherent stochasticity of the problem is so significant that the system being analyzed may not be predictable and/or engineerable. Figures 5 and 6 compare the LP approximation of the variance to that calculated by the benchmark for two test problems presented in the previous section – the first has a void fraction of 0.048 and the second a void fraction of 0.66. In both figures, we see that the benchmark estimate of the relative variance is small (very near zero for small void fraction), whereas the LP estimate starts at zero on the left edge of the problem and increases significantly toward the right edge of the slab. This indicates a serious inaccuracy in the LP approximation for the variance in these water/void problems. In fact, the LP estimate of the variance is substantially incorrect for many problems of practical interest, and will be the subject of future research.

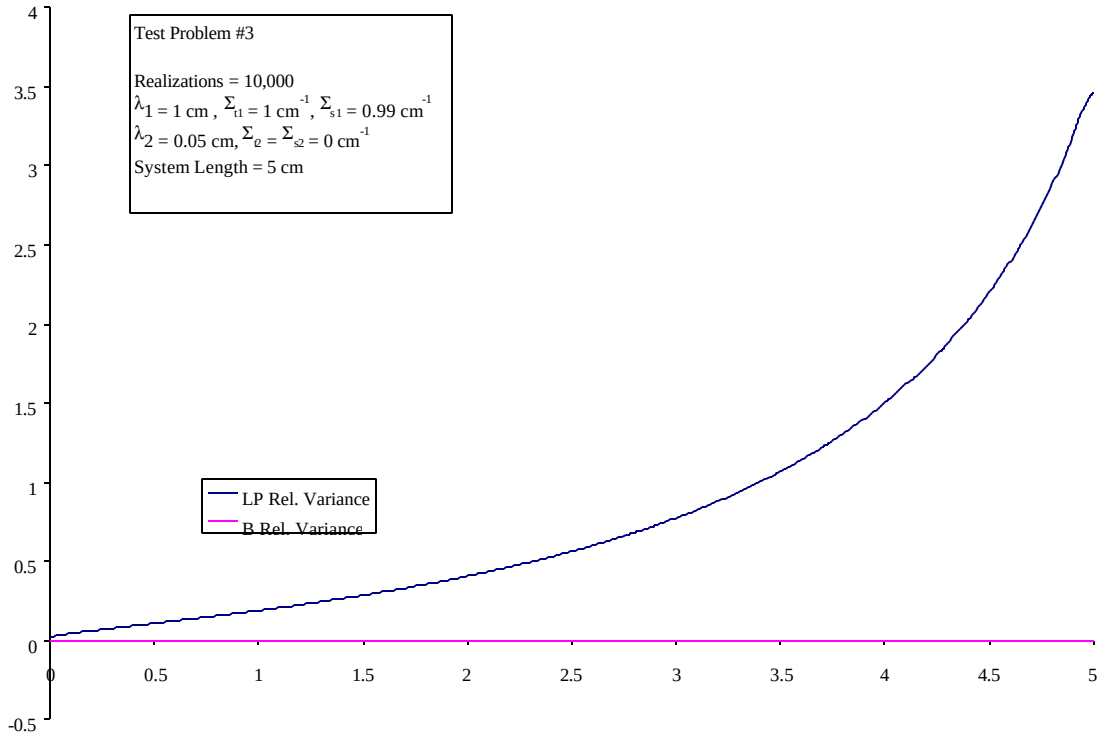


Figure 5: Relative variance in scalar flux for Test Problem #1

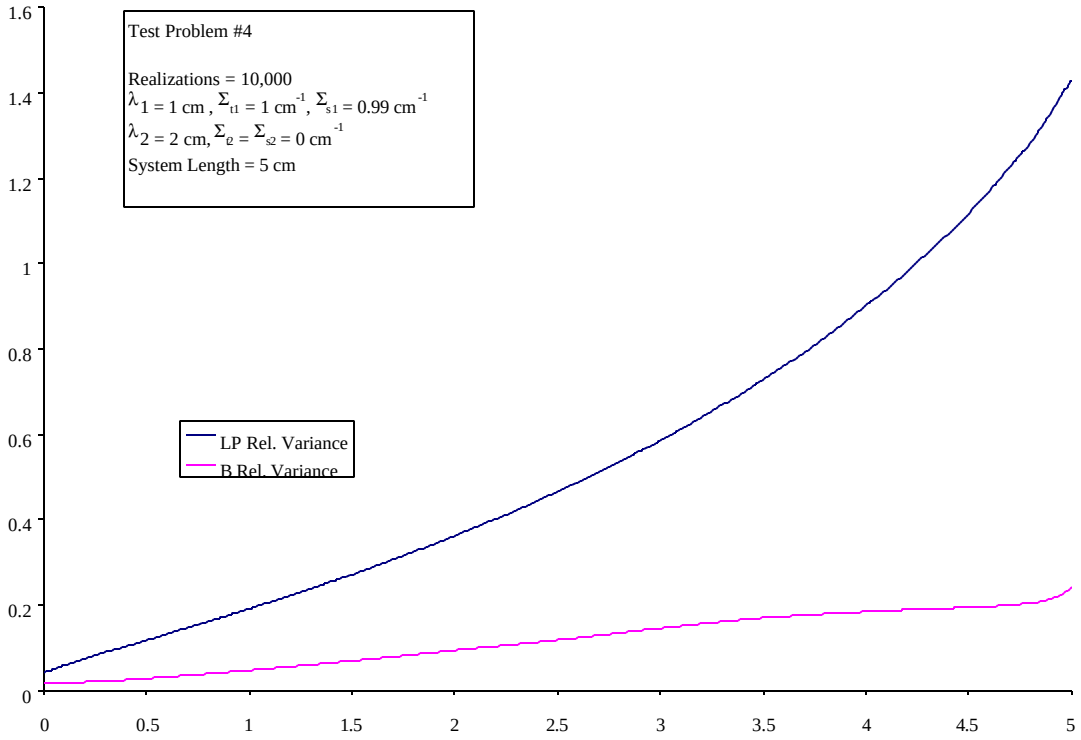


Figure 6: Relative variance in scalar flux for Test Problem #4

A full conference paper is in preparation containing a complete description of these findings [8] and it will be submitted to PHYSOR 2004 in Chicago, IL.

References

1. Q. Wu, S. Kim, M. Ishii, and S.G. Beus, "One-group interfacial area transport in vertical bubbly flow," Int. J. Heat & Mass Transfer, Vol. 41, Nos. 8-9, pp. 1103-1112, 1998.
2. G. Kocamustafaogullari and M. Ishii, "Foundation of the interfacial area transport equation and its closure relation," Int. J. Heat and Mass Transfer, Vol. 38, No. 3, 481, 1995.
3. Palmer, T.S. and Wu, Q., "Year 1 Progress Report - Improvements in Neutronics/Thermal-Hydraulics Coupling in Two-Phase Flow Systems Using Stochastic-Mixture Transport Models", DOE NEER Project DE-FC07-00ID13961, submitted to DOE July 1, 2001.
4. Bittle, w. and Palmer, T.S., "Criticality in Two-Phase Coolant/Fuel Lattices: An Investigation of the Accuracy of the Atomic Mix (Void Fraction) Assumption", accepted summary, PHYSOR 2002, Seoul, South Korea, October, 2002.
5. Olsen, G., private communication, 2003.
6. Ching, B. and Palmer, T.S., "An Acceleration Scheme for Binary Stochastic Mixture Deterministic Transport in Slab Geometry", Proceedings of the Amer. Nucl. Soc. International Meeting on Mathematical Methods for Nuclear Applications, September, 2001, Salt Lake City, UT.
7. Larsen, E.W., private communication, 2003.
8. Davis, I., and Palmer, T.S., "Levermore-Pomraning and Atomic Mix vs. Benchmark Calculations: Chunks in a Void", in preparation for PHYSOR 2004, Chicago IL.

Presentations

1. Davis, I., and Palmer, T.S., "Levermore-Pomraning and Atomic Mix vs. Benchmark Calculations: Chunks in a Void", Presented to CCS-4 at Los Alamos National Laboratory, August 7, 2003.
2. Davis, I., and Palmer, T.S., "Levermore-Pomraning and Atomic Mix vs. Benchmark Calculations: Chunks in a Void", Presented to Bettis Laboratory, September 9, 2003.

Appendix A: Bittle and Palmer PHYSOR 2002 summary (accepted but withdrawn from publication by the primary author for personal reasons)

Criticality in Two-Phase Coolant/Fuel Lattices:
An Investigation of the Accuracy of the Atomic Mix (Void Fraction) Assumption

whitney Bittle and Todd S. Palmer
Department of Nuclear Engineering and Radiation Health Physics
Oregon St. University
116 Radiation Center
Corvallis, OR 97331-5902

INTRODUCTION

Using a variety of flow visualization techniques, thermal/hydraulic researchers have been gathering more detailed information about bubble size distributions under a variety of flow conditions[1]. The primary purpose of this research is to improve two-phase fluid dynamic modeling of the reactor. However, the presence of this data suggests the following question: given more detailed information about the spatial distribution of the coolant mixture, could this information be used to obtain more accurate neutronic calculations? In BWRs (and PWRs under accident conditions), two-phase mixtures are typically treated using an "atomic mix" approximation; i.e. the spatial distribution of the two phases is ignored, and cross-sections are determined by a volume fraction weighting of the densities of each phase. Researchers have proposed improving upon the atomic mix model using stochastic mixture transport equations, but to assess the necessity of this considerable expense, it is important to compare the results from the atomic mix model to benchmark (spatially resolved liquid/vapor regions) transport calculations. In this paper, we discuss preliminary findings of the effect of the atomic mix assumption on the multiplication factor (k). Three dimensional pin cell Monte Carlo transport simulations were used to estimate the difference in k between the atomic mix and spatially resolved results. Our results show that at large void fractions (>30%), there is a significant difference between the two approaches.

METHODOLOGY

A typical BWR fuel pin[3] was modeled using MCNP4b with reflecting boundaries to create an infinite lattice representation. Calculations of k using the atomic mix (AM) approximation were preformed with 10^8 neutrons at void fractions of 10, 20, 30, and 40 percent by reducing the density of water accordingly. For example, at 30% void the density of water within the coolant channel would be reduced from 1 g/cm^3 to 0.7 g/cm^3. Since there is no neutron leakage in an infinite model, a uranium enrichment of 1% was used for the fuel. This enrichment, which is considerably lower than that of typical BWR fuel, was chosen because it produces a multiplication factor of 1.0. Calculations of k ranged from 1.0374 at 10% void to 1.0134 at 40% with a standard deviation of 0.0001 ($0.014) in all cases.

Calculations with spatially resolved (SR) void/coolant interfaces were first preformed with a large, spherical void located in the center of the channel. The top and bottom reflecting boundaries were separated by the same distance for all void fractions to create a repeating cell of constant volume, and the sphere volume was varied to model the different void fractions. The pin dimensions and fuel enrichment of the spatially averaged model were used. Calculations of k from this model at 10^7 neutrons ranged from 1.0377 at 10% void to 1.0162 at 40% with a standard deviation of 0.0004 ($0.057). While the results of the two models are within one standard deviation for 10% void, the difference between the AM and SR results increased as the void fraction increased – a difference in k of 0.0028 ($0.40) was calculated at 40% void. The results of the large bubble model show a substantial difference in k at high void fractions, but are still not representative of the actual geometry of void distribution in a nucleate boiling regime.

To determine whether bubble size was a significant factor in the calculation of the multiplication factor, the calculations described in the previous section were performed with *N* bubbles of equal volume, distributed as uniformly as possible, where *N*=2, 3, 4, … , 15, 20, 24, 29, 42, 49, 64, and 92 bubbles. For example, at 40% void, 15 identical bubbles each have a diameter of 2.75 mm, and 92 bubbles each have a diameter of 1.12mm, a reasonable lower bound on bubble size. Table 1 shows the range in the multiplication factor calculated from the different bubble sizes, which clearly indicates that bubble size has an effect on multiplication factor.

	Atomic Mix			**Spatially Resolved**			
	k	**High** k	**Low** k	High Δk	High Δ$	Low Δk	Low Δ$
10%	1.037	1.038	1.036	0.0005	0.07	-0.0012	-0.17
20%	1.034	1.036	1.034	0.0017	0.24	-0.0004	-0.06
30%	1.027	1.032	1.028	0.0048	0.69	0.0006	0.09
40%	1.015	1.02	1.018	0.0049	0.7	0.0025	0.36

Table 1: Comparison of Multiplication Factor (*k*) calculated by Atomic Mix (AM) and Spatially Resolved (SR) models.

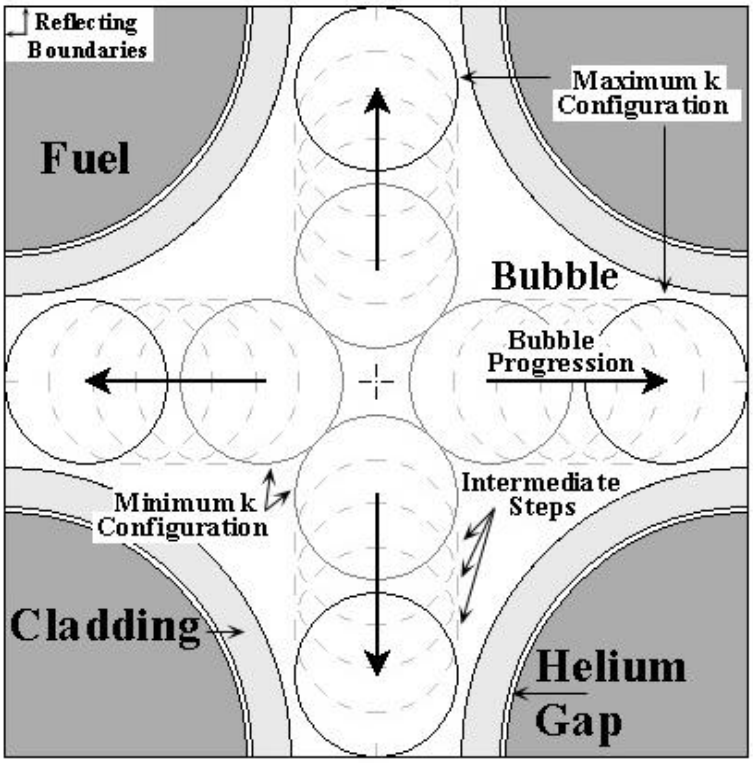


Figure 1: Pin cell configuration used in calculating significance of bubble position.

Another important consideration is whether bubble spatial distribution effects the multiplication factor. To investigate this we performed a series of calculations at a void fraction of 20% with four bubbles – this arrangement allowed the 3.66mm diameter bubbles to fit into the

3.70mm gap between two adjacent fuel pins. In the first calculation the four bubbles were clustered at the center of the channel (Figure 1), producing a k of 1.0345 (+/-0.0005), which is less than one standard deviation from the atomic mix value. In successive calculations the bubbles were slowly moved out from the center of the channel to the narrow gaps between adjacent fuel pins. While the bubbles remained near the center of the channel there was no significant change in the multiplication factor. However, when the bubbles were located between two adjacent fuel pins, k increased up to a maximum of 1.0361 (+/-0.0005), which is a change of $0.23. From these calculations it becomes apparent that the location of bubbles as well as their size is important to the calculation of the multiplication factor.

CONCLUSIONS

Our MCNP4b calculations indicate that in the region of a BWR core where bubbly flow occurs, using the atomic mix treatment for the coolant may result in inaccuracies in the multiplication factor. It is important to note that to correctly evaluate the accuracy of the atomic mix model, it should be compared to the ensemble-average results sampled from the true bubble size and position distributions. We are currently incorporating this sampling into our calculations and will include these results in the full paper.

REFERENCES

1. Q. Wu, M. Ishii, and J. Uhle, "Framework of Two-group Model for Interfacial Area Transport in Vertical Two-phase Flows," Proceedings of the 1998 American Nuclear Society Winter Meeting, Washington, D.C. (1988).
2. G.C. Pomraning, "Transport Theory in Discrete Stochastic Mixtures," preprinted version for review (1999).
4. J.J. Duderstadt and L.J. Hamilton, **Nuclear Reactor Analysis**, John Wiley & Sons, Inc. (1976).
3. J. F. Briesmeister, editor, "MCNP – a General Monte Carlo N-Particle Transport Code," Los Alamos National Laboratory Report, LA-12625-M (1997).

Appendix B: Viewgraphs from presentation to Los Alamos National Laboratory CCS-4 entitled "Levermore-Pomraning and Atomic Mix vs. Benchmark Calculations: Chunks in a Void"

Slide 1

Levermore-Pomraning and Atomic Mix vs Benchmark Calculations: Chunks in a Void

Todd Palmer and Ian Davis

Department of Nuclear Engineering and Radiation Health Physics

Oregon State University

LANL - 8/7/03

Slide 2

Several transport problems consist of materials mixed randomly in a void (or near-void)

- **Neutrons in pebble-bed reactors**
- **Neutrons in two-phase water/steam mixtures**
- **Electrons in the lung (tissue and air)**
- **Neutrons/gammas in superheated drop detectors**

Slide 3

This is a special class of mix problem…

- **Microscopic cross-sections are the same in each material**
- **Number density is a stochastically varying quantity**
- **To investigate these problems we:**
  - Choose σ_t and σ_s ,
  - Choose the slab size,
  - Fix non-void mean chord length at 1 cm,
  - Choose void mean chord length

Slide 4

What are our options for stochastic mix transport?

- **Benchmark calculations**
  - Generate realizations of the mixing statistics, solve transport problem, repeat
  - Compute ensemble average quantities of interest
  - If one transport problem is expensive, imagine 10000 of them?
- **Atomic mix**
  - The easy way out…
- **Direct incorporation into Monte Carlo**
  - One more distribution to sample from…
- **Approximate models**
  - Ensemble average the transport equation BEFORE solving it.
  - Coupled transport equations – yield estimates of ensemble average directly
  - Solve with deterministic or Monte Carlo

Slide 5

Previous studies have compared various models to benchmark calcs.

- **Adams, Larsen and Pomraning – 1989**
  - Rod and slab geometries, transmission and reflection probabilities
  - LP model vs. benchmarks – ensemble average only (no variance)
  - Deterministic calculations
- **Zuchuat, Sanchez, Zmijarevic and Malvagi – 1994**
  - Slab geometry, flux and trans./reflect. probabilities
  - LP and two other models – ens. avgs., benchmark variances
  - Deterministic calculations
- **Haran, Shvarts and Thieberger – 2000**
  - 2D benchmarks, trans./reflect. Probabilities
  - Monte Carlo
  - Adjusted mixed cross-sections to match benchmarks

Slide 6

Previous studies…

- **Donovan and Danon – 2003**
  - Constant radius 2D disks, 3D spheres in background material
  - Transmission and reflection probabilities
  - Monte Carlo calculations

Slide 7

A couple of things have been overlooked…

- **How good is atomic mix for these problems?**
  - None of the previous papers have compared models, atomic mix and benchmarks.
- **How good is LP for these problems?**
- **How big are the variances in these calculations?**
  - Large variances ⟶ un-engineerable systems (I know it's not a word)
- **How accurate are LP estimates of variance for these problems?**
  - Larsen (2003, to appear) has derived an approximate model for calculating the variance in the ensemble average flux

Slide 8

LP equations

$$m\frac{\partial}{\partial x}(p_i y_i) + s_{t,i} p_i y_i(x,m) = \frac{s_{s,i}}{2} p_i f_i + \frac{p_i Q_i}{2} + |m|\left[\frac{p_j y_j}{l_j} - \frac{p_i y_i}{l_i}\right]$$

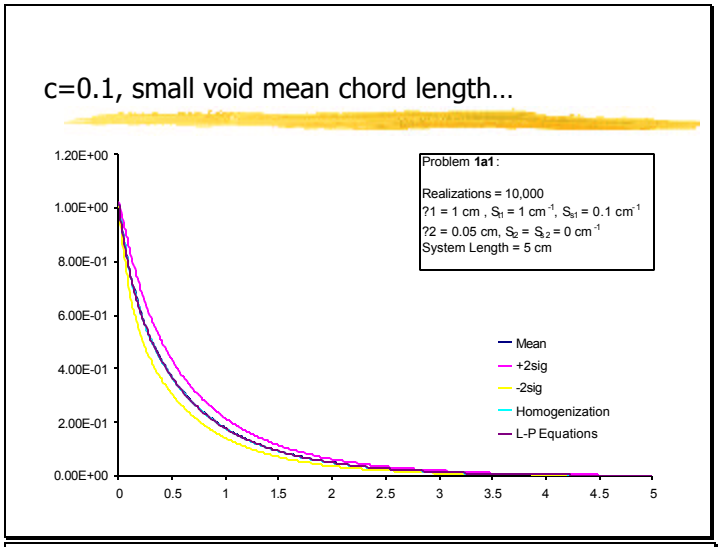
- **Two coupled equations for "material average" angular fluxes**
- p_i **= probability of finding material i at position x**
- **Approximate interface transfer term (much like two-phase flow modeling)**
- **Relatively easy to derive**
- **Ensemble average flux =** $p_i \psi_i + p_j \psi_j$

Slide 9

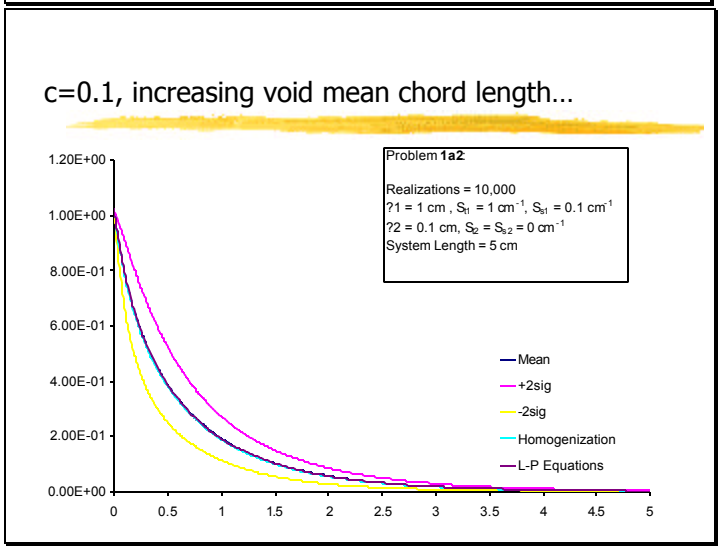
Problem matrix

- **c = 0.1, 0.5, 0.99**
- **X = 5 cm, 10 cm, 100 cm**
- l_1 **= 1.0 cm**
- l_2 **(void) = 0.05 cm, 0.10 cm, 1.0 cm, 5.0 cm**
- $s_{t,1}$ **= 1.0 cm^{-1}**
- **Driven on the left by an isotropic incident angular flux of 1**

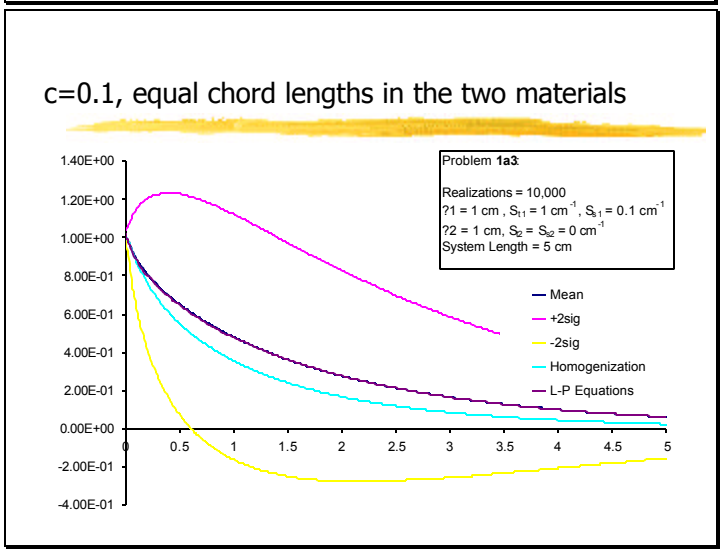
Slide 10



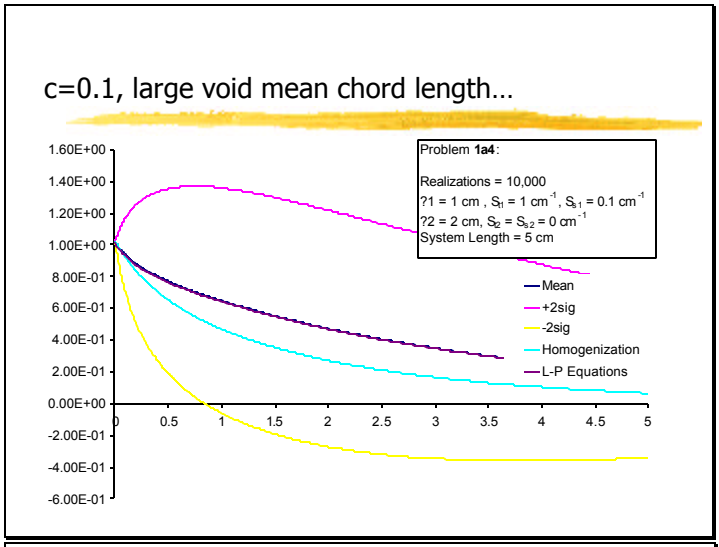
Slide 11



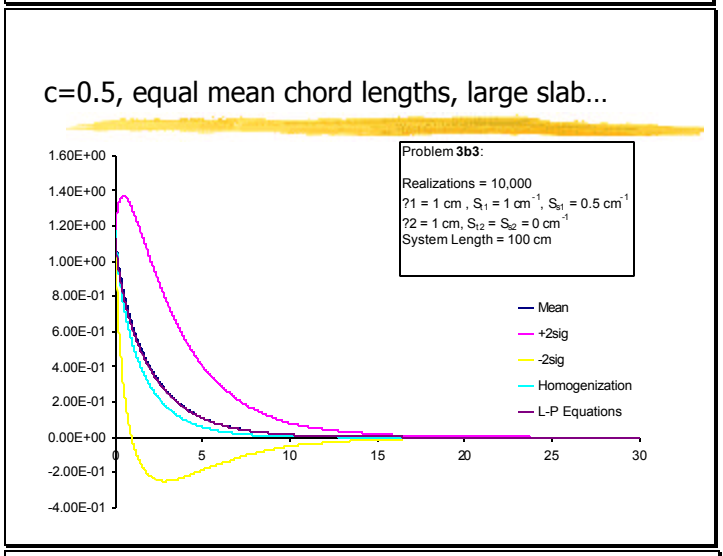
Slide 12



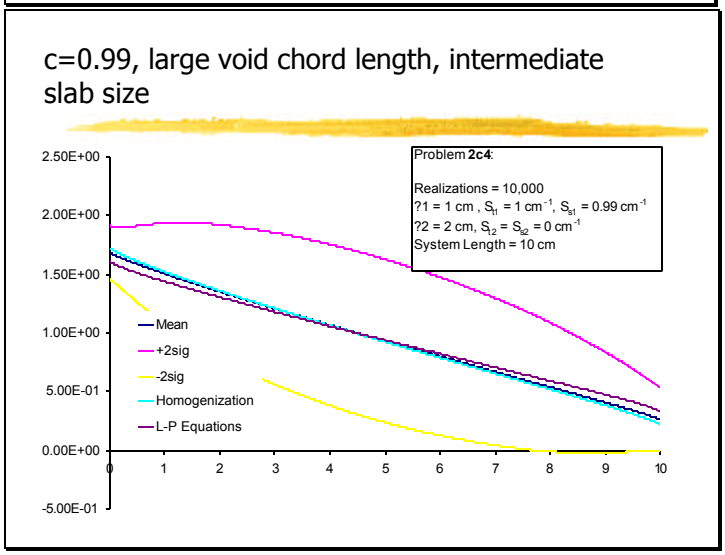
Slide 13



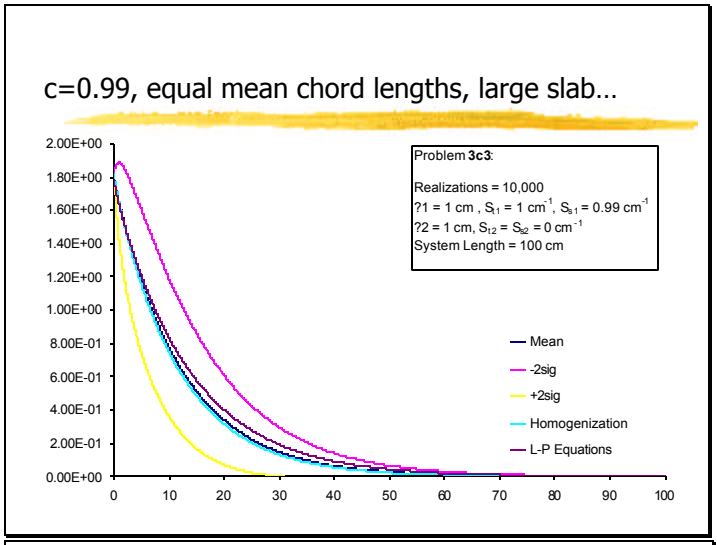
Slide 14



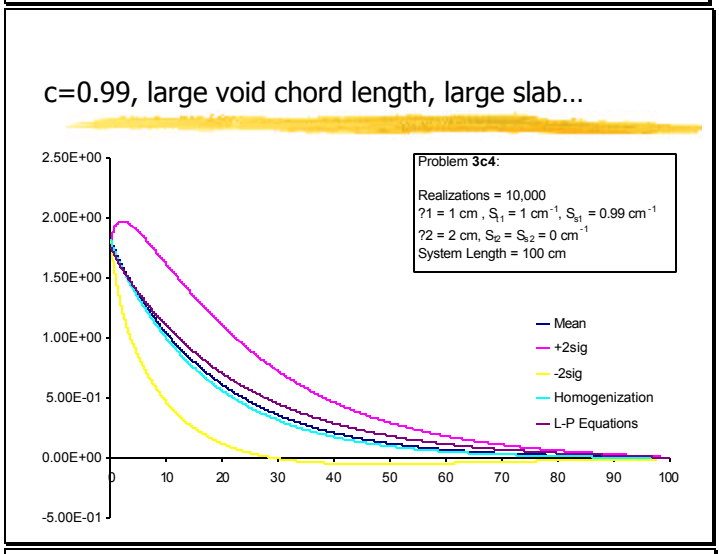
Slide 15



Slide 16



Slide 17

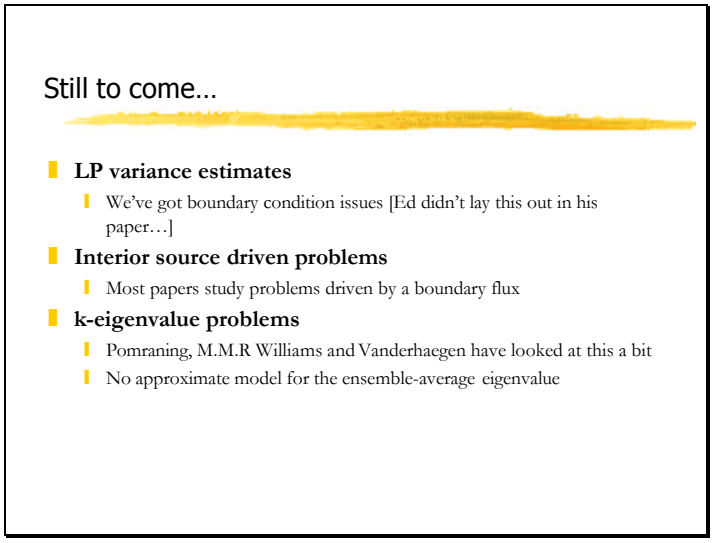


Slide 18

General trends

- **Atomic mix**
  - Accurate when λ_{void} is small relative to $\lambda_{non\text{-}void}$, independent of scattering ratio
  - When $\lambda_{void} >= \lambda_{non\text{-}void}$, can have flux errors as large as 100%
  - Generally within 1 σ of the benchmark results
  - As c approaches 1, atomic mix errors decrease
- **Levermore-Pomraning**
  - Exact in pure absorber, independent of chord lengths
  - As c increases, errors of ~10% in ens. avg. flux are observed for $\lambda_{void} >= \lambda_{non\text{-}void}$
  - As c approaches 1, LP can actually be worse than atomic mix (10% error vs 5%)
- **Benchmark variances**
  - As c increases, the variance in the ens. avg. flux increases
  - Can be as much as 100% of the mean!

Slide 19


Still to come…
LP variance estimates
We've got boundary condition issues [Ed didn't lay this out in his paper…]
Interior source driven problems
Most papers study problems driven by a boundary flux
k-eigenvalue problems
Pomraning, M.M.R Williams and Vanderhaegen have looked at this a bit
No approximate model for the ensemble-average eigenvalue

Appendix C: Year 1 Progress Report – Improvements in Neutronic/Thermal Hydraulic Coupling in Two Phase Systems Using Stochastic Mixture Transport Models

Improvements in Neutronics/Thermal-Hydraulics Coupling in Two Phase Systems Using Stochastic Mixture Transport Models

Nuclear Engineering Education and Research Program
U.S. Department of Energy

Year 1 Progress Report

July 1, 2001

Dr. T.S. Palmer, Associate Professor (palmerts@ne.orst.edu)
Dr. Q. Wu , Assistant Professor (qiao@ne.orst.edu)
Whitney Bittle, Graduate Research Assistant (bittle@engr.orst.edu)
Hong Tang, Graduate Research Assistant (tangh@engr.orst.edu)

Dept. of Nuclear Engineering
Oregon State University
116 Radiation Center
Corvallis, OR 97331-5902

Table of Contents

Introduction: Phase 1 Research

The goal of this project is to investigate the applicability of stochastic mixture transport models to the transport of neutrons in systems composed of fuel and two-phase coolant. This research is motivated by the observation that the treatment of any binary mixture of materials with substantially different cross-sections (i.e. different isotopes or densities) by a simple "volume-averaging" or "atomic mix" procedure is not a faithful representation of the physics and introduces errors. Researchers in the atmospheric transport community have recognized this, and are now using models for photon transport through cloudy atmospheres or plant canopies which incorporate, in an approximate way, statistical information about the distributions of the two materials in a binary mixture. These researchers were driven to find more accurate models because of mismatches between measured data and predictions from simulation codes.

The first research question we must ask is "Under what (if any) conditions is the atomic mix model inaccurate for reactor lattice neutron transport calculations?" The answer to this question lies in the comparison of "atomic mix" neutron transport calculations (in which coolant cross-sections are determined by a volume average of fluid and vapor phase cross-sections) with "benchmark" neutron transport calculations (calculations with the interface between the coolant fluid and vapor *explicitly resolved*). The majority of Phase 1 research (see Appendix I) is geared toward answering this question. Phase 1 involves three primary tasks:

A. Solution of simple benchmark problems to evaluate the importance of coolant heterogeneity in the calculation of neutron flux profiles and multiplication factor in two dimensions.
B. Determination of relevant thermal hydraulic parameters describing the degree of heterogeneity for different flow regimes.
C. Comparison of neutron transport calculations for homogeneous void treatment (void fraction only) and coupled stochastic transport treatment (void fraction and mean void diameter).

Progress on Task 1

Our proposal stated that we would first compare benchmark and atomic mix predictions of eigenvalue and spectra in simple geometries (one and two-spatial dimensions). We chose instead to use the MCNP4B Monte Carlo code to perform a large number of three-dimensional comparisons, primarily to investigate the change in eigenvalue. A proper comparison of the atomic mix model with a benchmark has these components:

- Choose the flow regime of interest (bubbly, annular, slug, …)
- Determine the distributions for the statistical parameters being considered – in this case the bubble size distribution (for a given flow regime, what is the probability of finding a bubble of a certain size) and void fraction spatial distribution (for a given flow regime, what is the spatial distribution of void)
- Sample from these distributions to generate a "realization" of the statistics
- Solve this problem for the data required (k-eigenvalue, energy spectrum)
- Repeat these steps until the statistics have been thoroughly sampled
- Compute average and standard deviation of results
- Compare these results with single atomic mix simulation using averaged input data.

As the determination of the bubble size and void fraction distributions was occurring simultaneously with the benchmark calculations, our preliminary analyses follow a somewhat different procedure:

- Choose a flow regime (bubbly, annular, slug, …)
- For a variety of physically realistic void fractions
  - Choose the number of bubbles in the channel
  - Assuming a uniform bubble size distribution, calculate the radius of the bubble
  - Uniformly distribute the bubbles in the channel
  - Solve the transport problem for each of these bubble size scenarios
- Compare each of these resolved calculations to the atomic mix calculation with averaged cross-section data.

The two important differences between this procedure and the one described on the previous page are the statistical sampling of the bubble size and void fraction distributions, and the averaging over many realizations. Our year two benchmark comparisons will utilize the distributions presented in this report.

Our MCNP4B calculations model a typical lattice assembly geometry for a boiling water reactor (BWR) was from data given in "Nuclear Reactor Analysis" by J.J. Duderstadt and L.J. Hamilton (Appendix H p.634). From this data a unit cell was created in MCNP4B having sides of 1.62 cm and one fourth of a fuel pin in each corner with an outer cladding radius of 0.625 cm, inner cladding radius of 0.5386 cm, and a fuel radius of 0.531 cm. The constituents of the zircalloy cladding used were 97.883% Zirconium, 1.5% Tin, 0.31% Iron, 0.2% Chromium, and 0.107% Nickel at a density of 6.51 g/cm^3. Pure helium at a density of 0.00016 g/cm^3 fills the gap between the fuel and the cladding. For purposes of comparison, the enrichment of the fuel was reduced to about 1% at a fuel density of 10 g/cm^3. This gives the channel a multiplication factor (k) of approximately 1.0. Since we are seeking the difference between the homogeneous and stochastic models it is not unreasonable to use an infinite lattice approximation.

Atomic mix cases – where the density of the water is reduced according to the void fraction – with 10^8 neutrons were simulated in MCNP4b to find a measurement of k. For example a void fraction of 30% was modeled by using a water density of 0.7 g/cm^3 which produced a *k* of 1.02690 with a standard deviation of 0.00014, or \$0.02. Results were generated for void fractions of 1% to 50% at each whole percentage; the largest standard deviation was 0.00015 (\$0.021).

For the resolved vapor-fluid interface calculations, a graphical trial-and-error method involving a scale drawing in Microsoft Paint was used to find the maximum diameter for a given number of equally sized spheres that would fit within the coolant region of the unit cell. For simplicity the centers of the spheres were required to lie on a plane perpendicular to the axes of the fuel pins. A cross-sectional view of the channel is shown in Figure 1.

The configurations for eight bubbles of various sizes are shown in Figure 2. When the bubble size is at its maximum, each sphere has a diameter of ~0.43 cm, which produces a void fraction slightly larger than 55% when reflecting planes are placed tangential to the tops and bottoms of the spheres. While leaving these two planes in place, the diameter of the spheres was reduced to 0.415016846 in order to achieve a void fraction of 50%. Since the bubbles are filled with steam, water at a density of 0.05598 g/cm^3 was placed inside the spheres. The process of reducing the diameter of the bubbles to decrease the void fraction was used to produce estimates of *k* for void fractions from 1% to 50% that could then be compared to the data calculated for the homogeneous case. As compared to the given homogeneous case, eight bubbles 0.350038764 cm in diameter give a void fraction of 30% and a *k* of 1.02954 ± 0.00046 (\$0.0657) after using 10^6 neutrons.

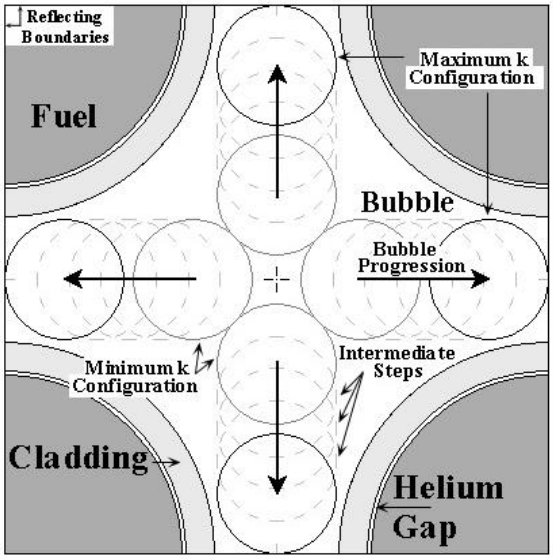
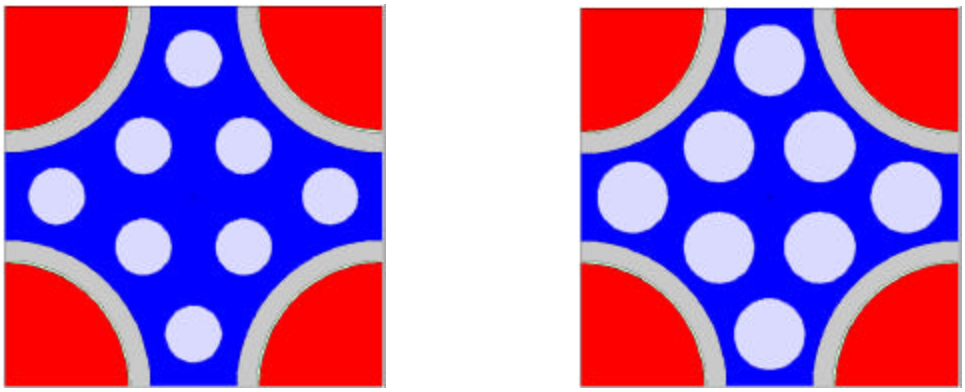
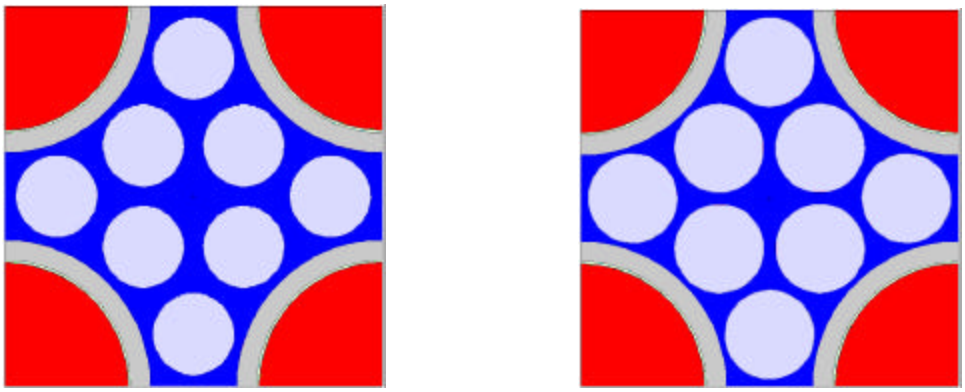


Figure 1: MCNP4B model of BWR lattice channel



(a) 10% (b) 20%



(a) 30% (b) 40%

Figure 2: Channel geometry with 8 bubbles and various void fractions.

Calculations with 10^6 neutrons were performed for one through fifteen bubbles at each whole void percent, from 1% to the maximum possible. In general, maximum void fractions greater than 40% were possible, with the exceptions of 2, 3, and 10 bubbles, which had maximums of 30%, 35%, and 37% respectively. At fifteen bubbles it became apparent that the difference in diameter between successive numbers of bubbles was becoming very small – 0.01 cm between the largest sizes of fourteen and fifteen bubbles (which had diameters of 0.2995 cm and 0.2894 cm). In addition the computing time necessary for each simulation was increasing due to the increase in cells in the model; one bubble at 30% void took 94 minutes for 10^6 neutrons, while fifteen bubbles at 30% void took 152 minutes for 10^6 neutrons. Therefore the next few runs were chosen based on an approximate change in initial bubble diameter of 0.02 cm, which leads to the unusual series of 24, 29, 42, 49, 64, 92. In addition simulations of each void percent were abandoned in favor of 10%, 20%, 30%, and 40% with 10^7 neutrons, which halved the error. At 92 bubbles the bubble diameter was 0.11 cm and the run time was 85:35. Due to time constraints further simulations were only performed at 30% void; the final calculation, at 383 bubbles, shows that there is still a large difference in *k* when the bubbles are only 0.05 cm in diameter.

Results

Tables 1-3 contain multiplication factors and Δk's for the void fraction/bubble size combinations simulated. The same data is represented graphically in Figures 3-5, along with the standard deviation in the calculations. In the 45%-35% void range the multiplication factor calculated with resolved fluid-vapor interfaces is markedly different than that calculated by the atomic mix model; the average difference in *k* for any number of bubbles was $0.74, $0.57, and $0.36 for 45%, 40%, and 35% void fraction, respectively. The 30%-20% range continues to show a decrease in the difference between the two models, dropping from an average of $0.25 at 30% to $0.12 at 25%, and then down to an average of only $0.05 at 20% which is lost within the error range of the calculations ($0.085). Unfortunately Figure 3 clearly illustrates that no useful information can be gained from the runs below 15% void since the error in the calculations is greater than the difference between the two models.

The 30% void calculations, augmented by the calculations at other void fractions, show that the moderation properties of a coolant channel with resolved vapor-liquid interfaces are substantially different than that of an atomically mixed channel. The average difference in the calculated multiplication factor was $0.25, which was three times higher than the standard deviation of the calculations. The more accurate calculations performed on higher numbers of bubbles continued to show an average of $0.25 even when the standard deviation was reduced to $0.04.

		Void Fraction (%)								
		45	**40**	**35**	**30**	**25**	**20**	**15**	**10**	**5**
Bubbles	**homo**									
	1	1.0769	1.0354	0.9903	0.9407	0.8853	0.8218	0.7467	0.6523	0.5177
	2				0.6358	0.5983	0.5554	0.5046	0.4408	0.3499
	3			0.5580	0.5300	0.4988	0.4630	0.4207	0.3675	0.2917
	4	0.5391	0.5184	0.4958	0.4710	0.4432	0.4114	0.3738	0.3266	0.2592
	5	0.4904	0.4715	0.4510	0.4284	0.4031	0.3742	0.3400	0.2970	0.2357
	6		0.4251	0.4066	0.3862	0.3635	0.3374	0.3065	0.2678	0.2125
	7		0.3956	0.3784	0.3594	0.3382	0.3140	0.2853	0.2492	0.1978
	8	0.4018	0.3863	0.3695	0.3510	0.3303	0.3066	0.2786	0.2433	0.1931
	9		0.3515	0.3362	0.3193	0.3005	0.2790	0.2535	0.2214	0.1757
	10				0.3083	0.2901	0.2693	0.2447	0.2138	0.1697
	11		0.3195	0.3056	0.2903	0.2731	0.2536	0.2304	0.2013	0.1597
	12	0.3189	0.3066	0.2932	0.2786	0.2621	0.2433	0.2211	0.1931	0.1533
	13	0.3066	0.2948	0.2820	0.2678	0.2520	0.2340	0.2126	0.1857	0.1474
	14	0.2952	0.2839	0.2715	0.2579	0.2427	0.2253	0.2047	0.1788	0.1419
	15	0.2853	0.2743	0.2623	0.2492	0.2345	0.2177	0.1978	0.1728	0.1371
	20	0.2480	0.2384	0.2281	0.2166	0.2039	0.1892	0.1719	0.1502	0.1192
	24	0.2277	0.2189	0.2094	0.1989	0.1872	0.1738	0.1579	0.1379	0.1095
	29	0.2057	0.1978	0.1892	0.1797	0.1691	0.1570	0.1426	0.1246	0.0989
	42		0.1648		0.1497		0.1308		0.1038	
	49		0.1516		0.1378		0.1203		0.0955	
	64		0.1327		0.1205		0.1053		0.0836	
	92		0.1117		0.1015		0.0886		0.0703	
	140				0.0830					
	217				0.0666					
	384				0.0500					

Table 1: Bubble diameters for the resolved vapor-liquid interface calculations

		Void Fraction (5%)								
		45%	**40%**	**35%**	**30%**	**25%**	**20%**	**15%**	**10%**	**5%**
Bubbles	**homo**	1.0037	1.0135	1.0211	1.0269	1.0314	1.0343	1.0363	1.0374	1.0376
	1		1.0163	1.0235	1.0282	1.0324	1.0349	1.0359	1.0377	1.0371
	2				1.0284	1.0325	1.0342	1.0365	1.0365	1.0379
	3			1.0226	1.0274	1.0320	1.0348	1.0367	1.0371	1.0373
	4	1.0078	1.0161	1.0225	1.0277	1.0318	1.0343	1.0367	1.0373	1.0370
	5	1.0109	1.0174	1.0239	1.0285	1.0322	1.0347	1.0362	1.0372	1.0372
	6		1.0189	1.0252	1.0293	1.0331	1.0346	1.0371	1.0370	1.0378
	7		1.0187	1.0236	1.0297	1.0333	1.0346	1.0366	1.0379	1.0371
	8	1.0104	1.0180	1.0236	1.0295	1.0321	1.0347	1.0369	1.0367	1.0383
	9		1.0179	1.0239	1.0294	1.0324	1.0346	1.0363	1.0378	1.0372
	10				1.0286	1.0317	1.0341	1.0360	1.0366	1.0378
	11		1.0180	1.0245	1.0282	1.0323	1.0345	1.0365	1.0371	1.0371
	12	1.0090	1.0166	1.0234	1.0286	1.0322	1.0345	1.0365	1.0362	1.0375
	13	1.0084	1.0176	1.0228	1.0281	1.0318	1.0354	1.0361	1.0373	1.0378
	14	1.0088	1.0172	1.0230	1.0290	1.0318	1.0341	1.0364	1.0369	1.0374
	15	1.0089	1.0174	1.0240	1.0281	1.0315	1.0353	1.0367	1.0376	1.0371
	20	1.0092	1.0184	1.0244	1.0298	1.0325	1.0346	1.0371	1.0382	
	24	1.0090	1.0167	1.0238	1.0278	1.0313	1.0337	1.0358	1.0376	1.0381
	29	1.0089	1.0168	1.0236	1.0286	1.0318	1.0350	1.0365	1.0377	1.0375
	42		1.0174		1.0287		1.0352		1.0371	
	49		1.0173		1.0289		1.0351		1.0373	
	64		1.0173		1.0287		1.0348		1.0373	
	92		1.0172		1.0284		1.0345		1.0372	
	140				1.0291					
	217				1.0290					
	384				1.0285					

Table 2: Multiplication factor (k) for the resolved vapor-liquid interface calculations

		Void Fraction								
		45%	**40%**	**35%**	**30%**	**25%**	**20%**	**15%**	**10%**	**5%**
Bubbles	**homo**	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
	1		0.400	0.340	0.179	0.143	0.091	-0.053	0.049	-0.077
	2				0.207	0.159	-0.007	0.031	-0.119	0.030
	3			0.213	0.067	0.099	0.069	0.054	-0.031	-0.047
	4	0.580	0.377	0.207	0.113	0.070	0.003	0.066	-0.007	-0.086
	5	1.019	0.557	0.396	0.233	0.124	0.067	-0.014	-0.016	-0.064
	6		0.777	0.586	0.339	0.254	0.050	0.116	-0.053	0.027
	7		0.744	0.354	0.397	0.274	0.043	0.043	0.074	-0.077
	8	0.957	0.646	0.357	0.377	0.104	0.066	0.086	-0.090	0.094
	9		0.641	0.396	0.363	0.144	0.047	0.001	0.059	-0.067
	11		0.649	0.484	0.189	0.131	0.026	0.039	-0.043	-0.074
	12	0.746	0.453	0.331	0.247	0.123	0.029	0.033	-0.160	-0.026
	13	0.664	0.594	0.244	0.176	0.060	0.154	-0.023	-0.011	0.029
	14	0.716	0.530	0.280	0.293	0.063	-0.026	0.017	-0.069	-0.039
	15	0.743	0.557	0.417	0.171	0.017	0.153	0.061	0.039	-0.077
	20	0.786	0.711	0.474	0.417	0.161	0.043	0.116	0.119	
	24	0.744	0.469	0.394	0.126	-0.003	-0.084	-0.073	0.031	0.060
	29	0.730	0.480	0.364	0.240	0.069	0.099	0.029	0.046	-0.016
	42		0.561		0.259		0.136		-0.034	
	49		0.553		0.281		0.114		-0.010	
	64		0.554		0.250		0.073		-0.011	
	92		0.530		0.209		0.030	-0.086	-0.029	
	140				0.319					
	217				0.300					
	384				0.230					
	Average	0.74063	0.56817	0.36286	0.24988	0.11723	0.05592	0.03109	-0.01272	-0.02562

Table 3: Δk between resolved vapor-liquid interface and atomic mix calculations

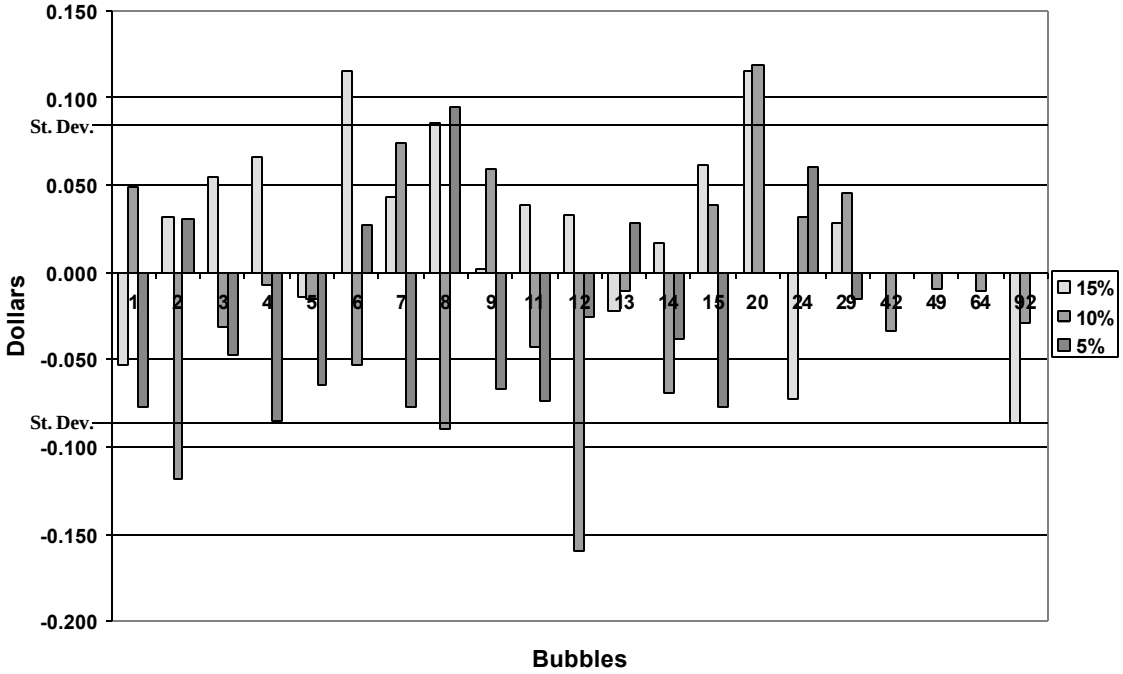


Figure 3: Δk (Resolved liquid-vapor interface vs. atomic mix) for small void fractions.

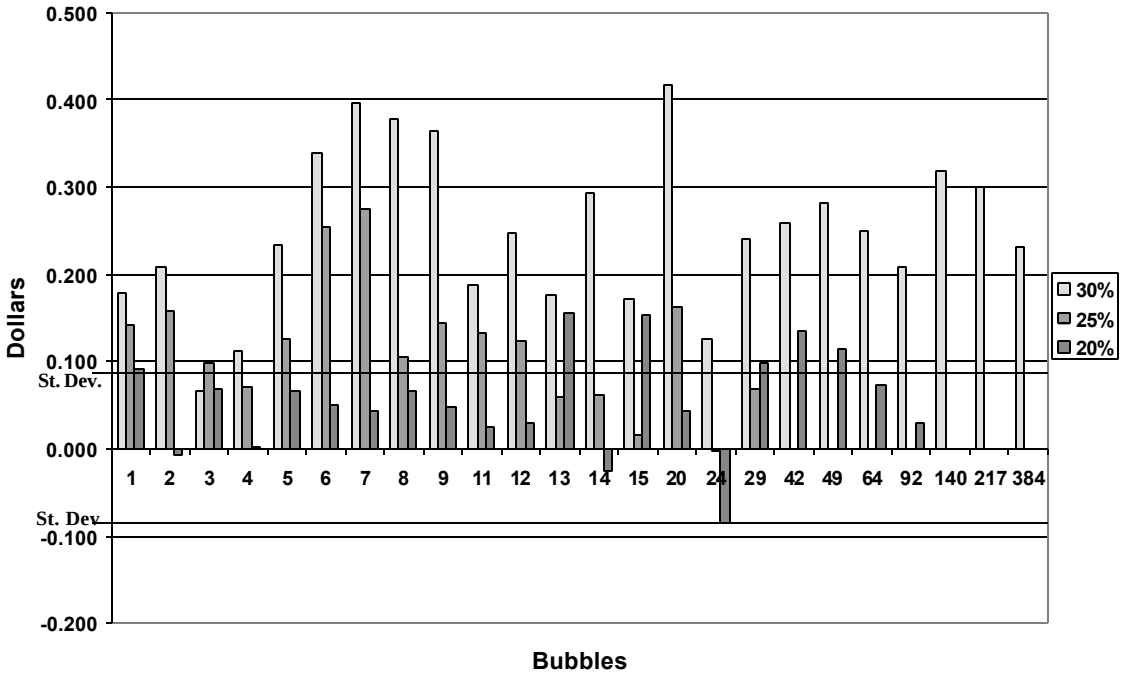


Figure 4: Δk (Resolved liquid-vapor interface vs. atomic mix) for intermediate void fractions.

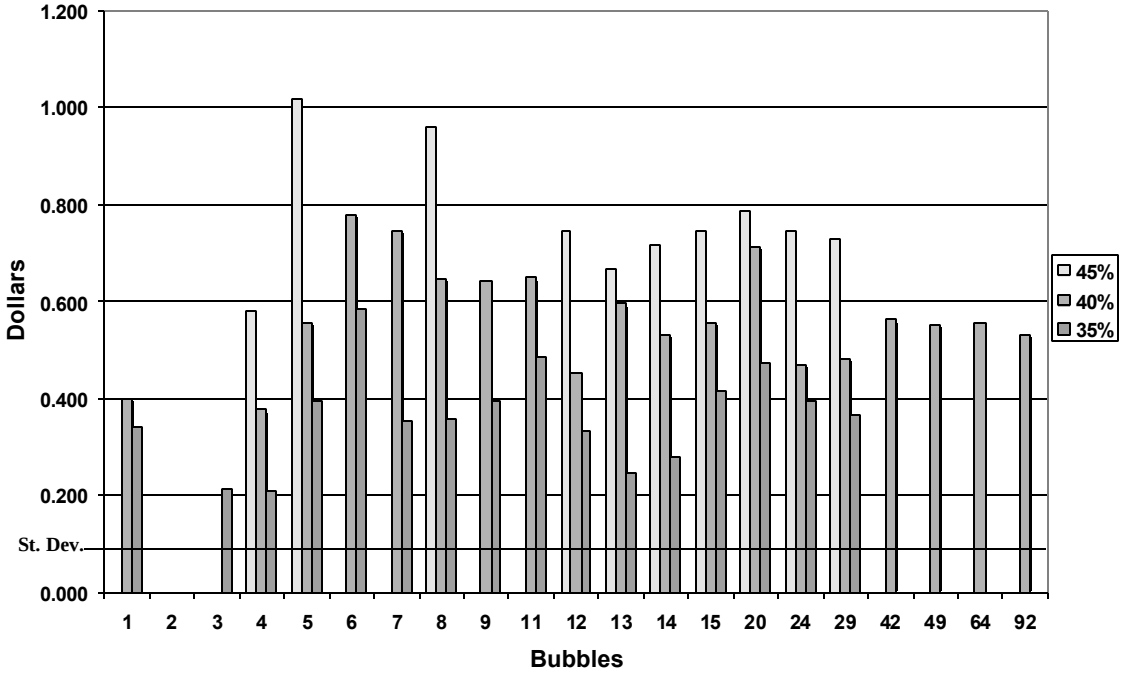


Figure 5: Δk (Resolved liquid-vapor interface vs. atomic mix) for large void fractions.

Progress on Task 2

The thermal hydraulic parameters describing the degree of heterogeneity for different flow regimes have been determined for bubbly, slug, and annular flow regimes. Generally, the bubble number density distribution function, $f(\mathbf{r}, V, t)$, is defined as the number of bubbles per unit mixture volume with the bubble volume between V and $V+\Delta V$ at a position $\mathbf{r}$ and a given time t. The "instantaneous" value of $f(\mathbf{r}, V, t)$ in fact should be a time-averaged value within certain time interval. Accordingly, the parameters of interest are defined by:

$$\text{Bubble Number Density: } n(\mathbf{r},t)=\int_0^\infty f(\mathbf{r},t,V)dV$$

$$\text{Local Average Void Fraction: } a(\mathbf{r},t)=\int_0^\infty f(\mathbf{r},t,V)VdV$$

$$\text{Local Bubble Volume-mean Diameter: } \overline{D}_V(\mathbf{r},t)=\left\{\frac{6\int_0^\infty f(\mathbf{r},t,V)VdV}{p\int_0^\infty f(\mathbf{r},t,V)dV}\right\}^{1/3}$$

As long as the particle number density distribution function, $f(\mathbf{r}, V, t)$, is given, those average parameters can be readily obtained from their respective definitions. Obviously, it depends on flow regimes due to the variations of bubble shape.
In the bubbly flow regime, bubbles are in spherical, elliptical or small cap shapes. For simplicity, spherical bubble shape is a rational approximation, which can greatly simplify the mathematical derivations. Since bubbles are highly dispersed in turbulent liquid, bubble size and the space coordinates are assumed to be independent of each other (experimental data of Wu et al. confirmed this claim [1]). The upper limit of bubble size follows the criterion of Kocamustafaogullari and Ishii [2]:

$$V_c=\frac{p}{6}\left[4\left(\frac{s}{g\Delta r}\right)^{1/2}\right]^3$$

The bubble size distribution should be within this limit. A typical distribution function is the upper-limit log-normal distribution function. However, the true distribution function depends on phase change rate, bubble nucleation mechanism, and bubble coalescence/breakage, which rely on the full solution of the two-fluid thermal-hydraulics model with the addition of interfacial area transport equation. Unfortunately, such a model capability is not available yet. In this study, we shall take the two approximate approaches. The first approach is to define an upper-limit log-normal distribution function throughout the bubbly flow regime. Subsequently, the void fraction increase due to vaporization can only boost the total bubble population. This artificial distribution function is effective to the validation of the proposed higher order Stochastic Mixture Transport Model, without involving the complexity of solving the fully coupled thermal-hydraulics equations. The second approach is to employ a uniform bubble size distribution function that allows the mean bubbly size change in the flow direction. In this case, a one-

dimensional thermal-hydraulics model can be applied along with the one-group interfacial area transport equation developed by Wu et al. [1].

The special variation of the distribution function, independent of the bubble size, depends on the heating arrangement. For near saturation boiling on nuclear fuel clad surface, bubbles intend to accumulate in the center core region, resulting in a center-peaking void distribution, except in the bubble incipient region where wall-peaking void distribution presents. It can be modeled by $(1-(r/R)^n)$ without loss its generality.

In the slug flow regime, bubbles are assumed to be of a lateral size close to the flow channel size. Small bubbles in the wake region are neglected. Therefore, the slug frequency plays a vital role in the analysis. Depending on the overall void fraction ($0.3<\alpha<0.8$), the slug frequency can be readily assigned in the proposed higher order Stochastic Mixture Transport Model.

In the annular flow regime, a thin liquid film attaches to the pipe wall and a small amount of liquid is dispersed in the vapor core in the form of droplets. As a approximation, only the liquid film is considered and the film thickness is obtained from void fraction.

References

1. Q. Wu, S. Kim, M. Ishii, and S.G. Beus, "One-group interfacial area transport in vertical bubbly flow," Int. J. Heat & Mass Transfer, Vol. 41, Nos 8-9, pp. 1103-1112 (1998).
2. G. Kocamustafaogullari and M. Ishii, "Foundation of the interfacial area transport equation and its closure relation," Int. J. Heat and Mass Transfer, Vol. 38, No. 3, 481 (1995).

Progress on Task 3

Task 3 is the comparison of benchmark calculations of BWR coolant channels with improved models of stochastic mixture transport. Our proposal indicated that we would develop a code in two-dimensions that would solve the binary stochastic mixture transport equations, leveraging our previous work in one dimension. After carefully evaluating the difficulty involved with writing a deterministic transport code capable of modeling fuel lattices, we decided instead to *obtain* a code which already solves multigroup k-eigenvalue transport problems in two-dimensions, and modify it to account for the binary mixture in the coolant.

The code we have obtained is called TALC, and it was written by Mike Zika as part of his Ph.D. thesis research at Texas A&M university. TALC solves the neutron transport equation in a general fuel assembly geometry using the long characteristics spatial discretization – the same spatial discretization used in the Studsvik of America code CASMO. We have the source code for TALC, and used the code to solve several test problems to assess its accuracy and efficiency.

Modifying this code to solve the coupled binary stochastic mixture transport equations requires that we develop a long-characteristics discretization of the coupled equations. Our previous research on solution techniques for these coupled equations suggests that transport sweeps become slightly more complicated. For example, if the discretization uses N fundamental unknowns per cell, then the within-cell matrix that must be solved is 2Nx2N. The long characteristics discretization yields computationally efficient transport sweeps because of the method's simplicity. The streaming plus collision operator is analytically inverted – in binary stochastic mixture transport, a set of two ODEs must be analytically inverted to perform the sweep. We are currently working on the development of the sweep equations for our improved version of TALC, and will be implementing these changes in year two.

Summary

We have made substantial progress on Task 1 (75% complete) and Task 2 (100% complete); however, we have much to accomplish in year two. It is likely that we will require a no cost extension to bring the project to completion. The modification of the TALC code is a substantial undertaking, and may require up to six months of additional time.

Appendix I: Proposed Research Plan

Our proposed research will take place in two phases. Phase 1 will have a duration of 12 months (April 1, 1999 – March 31, 1999) . The primary goal of the first phase is to establish the significance of the improvement in modeling two-phase coolant when using the stochastic mixture model.

Phase 1

The first task in Phase 1 involves the solution of simple, idealized, two-dimensional benchmark problems designed to point out differences in neutron flux profiles and multiplication factor values when comparing the homogeneous (or atomic mix) model with calculations that fully resolve the liquid-vapor distribution. These two-dimensional benchmark problems will be rectangular unit cell calculations, and will be solved with a numerical transport code that uses the Discrete-Ordinates angular differencing scheme, linear discontinuous spatial differencing, and two-group cross-section data for standard light water reactor fuel and coolant. The density difference between vapor and liquid will be varied to analyze the effect this has on differences between the homogeneous and stochastic mixture models. This work will be performed by T.S. Palmer and a graduate student under his direction.

Our second task involves the determination of relevant thermal hydraulic parameters describing the degree of heterogeneity for different flow regimes. Data available in from a variety of two parameter models will be gathered and translated into a form that can be used by a coupled, binary stochastic mixture transport code. Q. Wu and a graduate student under his direction will carry out this portion of the research.

Upon successful completion of our first two tasks, we will develop a two-dimensional coupled stochastic transport code (2-group, k-eigenvalue). This work will leverage code development efforts currently underway at Oregon St., which are currently being supported by a grant from Lawrence Livermore National Laboratory. We will then use this code to simulate neutron transport calculations for homogeneous void treatment (void fraction only), coupled stochastic transport treatment (void fraction and mean void diameter), and fully resolved liquid-vapor interface calculations. This work will be performed by T.S. Palmer and a graduate student.

Phase 2

Phase 2 will have a duration of 12 months and will begin following successful completion of Phase 1. The primary goal of phase 2 is to incorporate the stochastic mixture model into a reactor fuel assembly lattice code. For this portion of the project, we will modify a freely available integral neutron transport code (either collision probabilities or long-characteristics method) so that it can solve the coupled equations derived earlier. This code will then be used to generate assembly-flux-averaged cross-sections for a set of BWR benchmark problems. Assembly-flux-averaged cross-sections will also be generated using the homogeneous coolant model. Both sets of cross-sections will be used in a core simulator code and the results will be compared to each other and to measured data. In this way, the impact of the stochastic mixture model on the accuracy of core parameters can be evaluated.

Appendix II: Task Breakdown by Budget Period

Phase 1 Performance Period – June 1, 2000 to May 31, 2001
Phase 1 Funding - $97,802
Phase 1 – Phase 1 will have a duration of 12 months and will cover the following tasks:

D. Solution of simple benchmark problems to evaluate the importance of coolant

heterogeneity in the calculation of neutron flux profiles and multiplication factor in two dimensions.

E. Determination of relevant thermal hydraulic parameters describing the degree of heterogeneity for different flow regimes.
F. Comparison of neutron transport calculations for homogeneous void treatment (void fraction only) and coupled stochastic transport treatment (void fraction and mean void diameter).

Phase 2 Performance Period – June 1, 2001 to May 31, 2002

Phase 2 Funding - $110,699

Phase 2 – Phase 2 will have a duration of 12 months and will begin after Phase 1. Phase 2 will cover the following tasks:

A. Implementation of stochastic mixture transport model into lattice code.
B. Comparison of assembly-averaged data from stochastic mixture lattice code with homogeneous-coolant lattice code.
C. Incorporation of stochastic mixture lattice data into core simulator.
D. Evaluation of the impact of stochastic mixture assembly data on core parameters.